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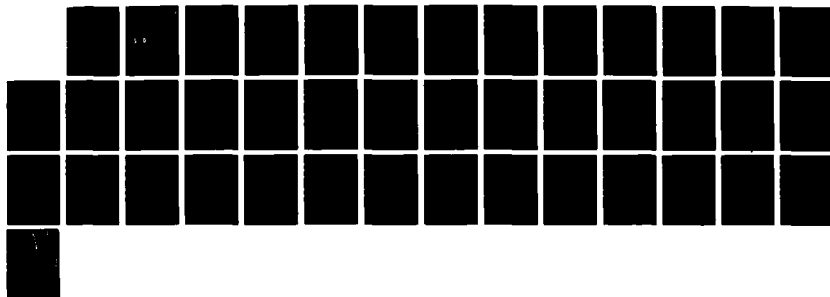
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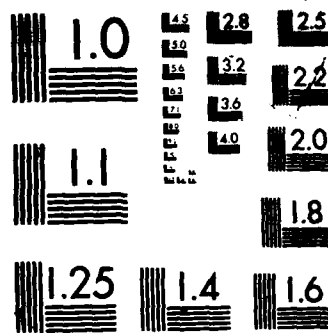
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Naval Research Laboratory

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**Photoionization of Atoms and Ions:  
Application of Time-Dependent Response  
Method Within the Density Functional Theory**

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<p>The photoionization cross-section of several atoms (Ar, Xe, Rn, Cs) and ions (Ne-like Ar, H-like and Li-like C) of experimental interest are calculated using the time-dependent response scheme within the framework of local density functional method (DFM). The cross-sections for rare gas atoms calculated using this method agree very well with the experimental data; whereas conventional independent particle model calculations do not. The polarization effect of the atom brought about by the incident time-varying radiation field is shown to be important in describing observed results. Unlike the independent particle model, this effect is treated adequately in the DFM.</p> <p>To study the effect plasma density and temperature on the photoionization cross-section, calculations were also done for the ions mentioned above at various densities and temperatures. For computational simplicity, a simplified model of self-consistent finite temperature DFM was used in which the long range part of the ionic potential was taken as the Debye-screened potential. These calculations were compared with the isolated ion calculations (without any plasma effect). With increasing plasma density, significant shifts of the ionization threshold as well as substantial modifications of photoionization cross-section are obtained. This points out the need for incorporating the effect of surrounding plasma in realistic modeling of atomic properties for dense plasmas.</p>					
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# Photoionization of Atoms and Ions: Application of Time-Dependent Response Method Within the Density Functional Theory

## I. INTRODUCTION

Accurate calculation of photoionization and photoexcitation cross-sections of atoms and ions are useful in a variety of investigations in plasma physics and atomic physics. It is particularly useful in the context of flashlamp photopumping schemes for x-ray lasers. Most of the existing calculations of photoionization cross-sections were done using the single electron or the independent particle model (IPA). In this model, the energy-levels, and wavefunctions of the atom or ion are first calculated using the Hartree-Fock (HF) method. The interaction of the incident electromagnetic radiation with the atom (or ion) is treated via the first order perturbation theory.

Comparison of experimental data with the IPA calculations shows that for some simple systems such as a neutral few electron atom (Lithium, for example), there is qualitative and sometimes quantitative agreement. However, for many electron atoms (Xenon, for example) and ions with a large number of bound electrons, substantial discrepancies are found between experimental and IPA-data.<sup>1</sup>

In our work, we used the time-dependent linear response approximation within the framework of the relativistic density functional method (DFM)<sup>2,3,4</sup> to treat the problem of photoionization. This method incorporates certain advantages over the HF-method. The HF-method is non-local and computationally very elaborate, whereas in the density functional method, one deals with a set of local equations only. This leads to computational simplicity. On the other hand, it is well known from extensive application of the density functional method, that fairly accurate atomic energy levels, wavefunctions etc. are obtained. The computational simplicity is even more apparent in the case of relativistic DFM versus relativistic HF-methods. In the DFM, correlation effects of

the bound electrons in the atom are accounted for in a simple way via the correlation potential. The Hartree-Fock method, on the other hand, does not take into account electron correlation, although it accounts for non-local exchange effects appropriately.

The independent particle method does not take into account the polarization effect of the atom brought about by the incident time-varying radiation field. In the linear response method within the density functional method, this is treated adequately - as will be seen from comparison with the experimental data. In most experimental situations, the incident radiation (from synchrotron sources or lasers) have field strengths small compared to the atomic field strengths. For those experimental conditions, the present model based on linear response is adequate and useful.

Calculations of photoionization and photoexcitation cross-sections and rates have a number of applications. For the photopumping scheme for x-ray lasers, these processes play a crucial role in contributing to a population inversion of excited ionic levels. As another example, computation of opacities of plasmas for diagnostic and target response effects require these data as input. In order to model the radiation spectra from hot plasmas (via detailed configuration rate equation technique, for example), the photoionization and photoexcitation data are required in addition to other bound-bound, bound-free and free-free processes. Accurate calculations are also necessary for interpreting experimentally available data on cross-sections. In view of these different applications, there is a need for realistic modeling of these processes in order to generate accurate data over a wide range of photon energy for a variety of atoms and ions. The present model provides such a tool and its usefulness will be discussed in subsequent sections.

The above discussion deals with the calculation of photoionization of isolated atoms or ions - that is, without the effect of the plasma environment. These effects are negligible for very low density plasmas. In many experimental situations, however, the plasma density can be quite high (for example, in laser produced plasmas). In those cases, additional effects due to screening shifts of energy levels and modification of wavefunctions and potentials for the ion embedded in high density plasmas have to be considered. In the later part of this report, we will present some results of photoionization cross-section of ions in a dense plasma medium and examine the modification of cross-sections due to the plasma environment.

## II. THE METHOD OF CALCULATION

The first part of the calculation is to generate the energy-level spectrum and the wavefunctions of the particular atom or ion of specific configuration. This is done by using the local density functional method. In order to treat many-electron atoms (with high  $Z$ ) appropriately, relativistic DFM equations were used. In this method, the following set of equation were solved self-consistently:

$$\left[ c \vec{\alpha} \cdot \vec{p} + c^2 \beta + u(\vec{r}) \right] \psi_i(\vec{r}) = E_i \psi_i(\vec{r}) \quad (1)$$

$$u(\vec{r}) = -\frac{Z}{r} + \int \frac{\vec{p}(\vec{r}') \cdot \vec{p}(\vec{r})}{|\vec{r}-\vec{r}'|} + \frac{\partial}{\partial \rho(\vec{r})} \left[ \rho(\vec{r}) \varepsilon_{xc}(\rho(\vec{r})) \right] \quad (2)$$

$$\text{and } \rho(\vec{r}) = \sum_i f_i |\psi_i(\vec{r})|^2 \quad (3)$$

In the above,  $\rho(\vec{r})$  is the electronic charge density of the atom,  $\vec{\alpha}$ 's are the Dirac matrices,  $f_i$ 's are the integral occupation factors corresponding to the number of electrons in each state  $\psi_i(\vec{r})$  with corresponding energy eigenvalue  $E_i$ . The atomic potential  $u(\vec{r})$



contains, in addition to the nuclear and the electrostatic Hartree term, a contribution arising from the electron exchange and correlation effects. Let us note that the use of integer occupation factors  $f_i$ 's for the given configuration distinguishes this model from the "average atom model" where the occupation factors are taken to be those given by the statistical Fermi distribution function.

The orbital functions are four-component spinors. They are split into major and minor components:

$$\psi(\vec{r}) = \begin{pmatrix} \psi^1(\vec{r}) \\ \psi^2(\vec{r}) \end{pmatrix} = \begin{pmatrix} (A(r)/r) i^l \alpha_{jlm}(\vec{r}) \\ (B(r)/r) i^{l'} \alpha_{j'l'm}(\vec{r}) \end{pmatrix} \quad (4)$$

where A and B are major and minor components of the radial functions and  $\alpha_{jlm}$  and  $\alpha_{j'l'm}$  are two-component Pauli spinors with the indicated numbers. The various quantum numbers are related by

$$l' = l + S, j' = l + 1/2, S = l' - 1/2, K = -S(j + 1/2); S = \pm 1 \quad (5)$$

The differential equations for A and B (in matrix form) are:

$$\frac{d}{dr} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} -K/r & (u - E - c^2)/cs \\ - (u - E + c^2)/cs & K/r \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \quad (6)$$

In Eq. (2),  $\epsilon_{xc}$  is the exchange-correlation energy of the electrons. In actual calculation, Gunnarsson-Lundquist (G-L) form<sup>3</sup> for exchange-correlation energy and potential was used. It is well known that reliable atomic data is obtained from the use of G-L exchange-correlation. Equations (1) - (6) are solved numerically to self-consistency to obtain the wavefunctions  $\psi_i$ 's, the binding energies of each orbital  $E_i$ , the atomic charge density  $\rho(\vec{r})$  and the self-consistent potential  $u(\vec{r})$ .

Now consider the effect of an incident time-varying radiation field  $E(t) = E_0 e^{i\omega t}$  on the atom. It induces a time-dependent atomic density deviation,  $\delta\rho(\vec{r}, t)$ , causing a time-dependent polarization effect. For the linear response method used here, it is convenient to work with the Fourier transform:

$$\delta\rho(\vec{r}, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \delta\rho(\vec{r}, \omega) e^{-i\omega t} d\omega \quad (7)$$

The net induced density due to the external plus the induced potential is

$$\delta\rho_{ind}(\vec{r}, \omega) = \int \chi(\vec{r}, \vec{r}', \omega) [V_{ext}(\vec{r}, \omega) + V_{ind}(\vec{r}, \omega)] d\vec{r}', \quad (8)$$

where the induced potential is given by

$$V_{ind}(\vec{r}, \omega) = \int \frac{\delta\rho(\vec{r}', \omega)}{|\vec{r} - \vec{r}'|} d\vec{r}' + \frac{\partial V_{xc}(\rho(\vec{r}))}{\partial \rho(\vec{r})} \delta\rho(\vec{r}, \omega) \quad (9)$$

The response function is given by

$$\begin{aligned} \chi(\vec{r}, \vec{r}', \omega) = & \sum_i f_i \psi_i^*(\vec{r}) \psi_i(\vec{r}') G(\vec{r}, \vec{r}', E_i + \omega) \\ & + \sum_i f_i \psi_i(\vec{r}) \psi_i^*(\vec{r}') G^*(\vec{r}, \vec{r}', E_i - \omega) \end{aligned} \quad (10)$$

and thus involves the wavefunctions and energy levels of the atom. The Green's functions are solutions of the inhomogeneous Dirac equation

$$(c\vec{\alpha} \cdot \vec{p} + c^2\beta + u(r) - E) G(\vec{r}, \vec{r}', E) = -\delta(\vec{r} - \vec{r}') \quad (11)$$

In actual calculation, angular decomposition of the Green's function in terms of spherical harmonics is done (Appendix I) and the radial part is treated separately.

The frequency dependent polarizability  $\alpha(\omega)$  is the ratio of the induced dipole moment to the external field:

$$\alpha(\omega) = - \frac{e}{E_0} \int Z \delta \rho(\vec{r}, \omega) d\vec{r} \quad (12)$$

Note that  $\alpha(\omega)$  like  $\delta \rho(\vec{r}, \omega)$  is complex. The induced density deviation (and also the corresponding induced potential) can have a phase difference with respect to that of the applied external field. Once  $\alpha(\omega)$  is determined, the photoabsorption cross-section  $\sigma(\omega)$  of the atom is obtained from:

$$\sigma(\omega) = \frac{4\pi\omega}{c} \text{Im } \alpha(\omega). \quad (13)$$

### III. PARTIAL CROSS-SECTION

In order to see the connection with the IPA-model, consider the partial cross-section due to photoionization from a specific bound state  $\psi_i(\vec{r})$  to a final continuum state  $\psi_f(\vec{r})$ .

The initial atomic state is represented as

$$\psi_i(\vec{r}) = \frac{U_{nl}(r)}{r} Y_L(\hat{r}) \quad (14)$$

and the final continuum state with wavevector  $\vec{k}$  and energy  $\epsilon$  as

$$\psi_f(\vec{r}) = 4\pi \sum_{L'} A_{1,i}^{L'} \frac{P_{\epsilon L'}(r)}{r} Y_{L'}^*(\hat{k}) Y_{L'}(\hat{r}) \quad (15)$$

The complex coefficients  $A_{1,i}^{L'}$ 's are found by requiring  $\psi_f(r)$  to behave asymptotically as an incident plane wave plus a spherical wave. Then the partial cross-section  $\sigma_{nl}$  is shown to be

$$\sigma_{nl}(\omega) = 2(2l+1) \alpha \hbar \omega \sqrt{\epsilon} a_B^2 \quad (16)$$

$$\times \sum_{L'} |A_{1,i}^{L'}|^2 \langle 100 | 1'0 \rangle^2 \left| \int P_{\epsilon L'}(r) V^{SCF}(r, \omega) U_{nl}(r) dr \right|^2$$

where  $\langle 1\ 100 | 1'0 \rangle$  is a Clebsch-Gordon coefficient.

In (16),  $v^{SCF}(r, \omega)$  is a frequency dependent complex self-consistent potential. Note that, if  $v^{SCF}(r, \omega)$  is replaced by the usual dipole moment operator, one obtains the conventional or independent particle approximation (IPA) result. In actual calculations, both bound and continuum wavefunctions are generated numerically using the Numerov method for integrating the Dirac equation. Let us also note that the real and imaginary parts of the self-consistent field contributes to the partial cross-section without interference. Computations were performed for both the conventional independent particle model and the time-dependent linear response to density functional method for comparison purposes.

#### IV. RESULTS

In Fig. 1, results of computed photoionization cross-section for neutral xenon is plotted as a function of photon energy near the 4d-threshold. The drastic difference between the results obtained from the time-dependent response method (curve A) and from conventional IPA-model (curve B) is clear. The IPA-model does not reproduce the experimental values<sup>5</sup> at all whereas the present time-dependent model agrees very well with the experimental data over this entire range of photon energy from 5 to 10 Ryd., including the peak at about 7 Ryd. In that energy range, the IPA cross-section shows a rapid decrease - in contrast to the experimental data.

The primary physical reason for this difference in the two models arise from the polarization effect of the atom subjected to the incident radiation. In the case of xenon, all of the 54 bound

electrons forming the atom participate in the polarization process (the outer ones contributing most). The external field is screened in the energy range 5-6 Ryd. (and again in the range 8.5 - 9.5 Ryd.), and is antiscreened in the intermediate 6-8 Ryd. range. The antiscreening effect produces a stronger effective field for the 4d-electron to photoionize, thereby enhancing the cross-sections somewhat in the intermediate energy range as seen in Fig. 1.

The 3s-partial cross-section for Argon is shown in Fig. 2. The experimental data<sup>7</sup> in the range of 30 - 65 eV are depicted by circles with the error bars. The conventional IPA-calculation (curve A) again does not show the experimentally seen variation at all. The present time dependent response method reproduces the observed variation including the experimental Cooper minimum at about 43 eV and is in good agreement with the measured cross-sections. The occurrence of the Cooper minimum is known<sup>1</sup> to be due to the vanishing of the matrix element between bound and continuum states at that photon energy. In the present time-dependent polarization model, the physical reason for the minimum is that the induced potential almost exactly cancels out the external field, reducing the effective field to almost zero.

The total cross-section for Argon atom as a function of the photon energy is plotted in Fig. 3, and compared with experimental data<sup>8</sup>. Comparison is also made of results obtained from Hartree-Fock (HF) length and velocity approximations by Kennedy and Manson<sup>6</sup>. We note that the time-dependent response model again best reproduces the experimental data. The HF-velocity approximation gives, for example, a cross-section twice as large at 40 eV whereas the HF-length result is six times larger than the experimental data at the same photon energy.

Good agreement with available experimental data for Ar, Ne, Kr and Xe suggests that reliable cross-sections can also be generated for higher-Z rare gas atoms such as Radon utilizing the time-dependent response model. For Radon ( $Z=86$ ), relativistic effects are significant. The Dirac equation approach in our model is therefore suitable. We performed self-consistent calculation for Radon and the computed total cross-section is plotted in Fig. 4 for the photon energy range 7-28 eV. The large difference between the results obtained from IPA-model and the present time-dependent response model is clearly seen from the graph. The large peaks due to the ionization from  $6p_{1/2} \rightarrow d_{3/2}$  in the IPA-model are masked significantly due to polarization effect incorporated in the time-dependent response model. No experimental data is available for the case of Radon. However, in view of the good agreement between experimental data and the results of time-dependent response model, it is expected that future experimental measurements for Radon in this photon energy range will be in close agreement with these calculated cross-sections.

The 6s partial cross-section for Cesium as a function of photon energy in the range of 4-8 eV is plotted in Fig. 5. In this particular case, there are significant differences in the two sets of experimental data<sup>9,10</sup> of the two groups, presumably due to uncertainties in vapor pressure measurement. Calculated value of partial cross-sections from the time-dependent model is in fair agreement with one set of observed data (Fig. 5). The effect of spin-orbit interaction is known to be significant for the 6s partial cross-section of Cesium. A more detailed theory should incorporate this effect. As seen from Fig. 5, the IPA-model shows a monotonic decrease of cross-section in this energy range in complete disagreement with the experimental data.

Ions of specific configurations such as Neon-like Argon are of interest for scaling to higher  $Z$  neonlike systems for x-ray laser research. No experimental data is available for these ions and thus the data have to be provided by theoretical calculations. The fact that the time-dependent response method is successful for generating accurate data for rare gas atoms suggests that reliable cross-sections can be generated for Ne-like Ar and other ions of interest. Computed results for Ne-like Argon are presented in Fig. 6 and compared with conventional IPA-calculations. The differences are smaller in this case, as expected, because the number of bound electrons for these ions is only ten. For these highly charged ions, these electrons are very tightly bound and thus do not participate as effectively in the polarization process.

The results presented above are for single atoms or ions without the effect of the plasma environment - as appropriate for very low density plasmas. For high density plasmas, however, effects due to screening shifts of energy levels, modification of wavefunctions of bound (particularly the upper levels) and continuum wavefunctions as well as potentials of the ion embedded in the plasma have to be considered.

For proper treatment these effects, the self-consistent density functional method (DFM) at finite temperatures<sup>11</sup> should be used. The application of this method requires iterative numerical solution of Schrodinger equation involving the complete set of bound and continuum wavefunctions for the multielectron ion and construction of effective potential inclusive of plasma screening and electronic exchange correlation effect in each iteration. For our present purpose, we adopted the following simplified approach for computational simplicity. For a given plasma density and temperature, we represent

the long range part of the effective potential in the Debye-screened form. The inner part of the effective potential was constructed by numerical integration of the Hartree term with the electron density distribution calculated using the bound state wavefunctions.

The results of our calculation for H-like and Li-like carbon ions are shown in figures 7-11. From fig. 7, we see, by comparing with isolated atom cross-sections, that the threshold for photoionization from 1s-level of H-like C shifts substantially (from 18 eV to about 15.2 eV) for Debye length  $\lambda_D = 2$  a.u. This is significant in the context of calculation of photoionization rates, which is calculated by integrating the cross-section weighted by the electron distribution function (usually the Maxwell-Boltzmann distribution) over the entire energy range. The calculated rates in the two cases would therefore be very different - as seen from fig. 7.

In fig. 8, the corresponding results of partial photoionization cross-section for H-like C is plotted. Fig. 9 shows the 3d-partial cross-sections of the same ion at two different plasma conditions ( $\lambda_D = 5$  and 2 a.u.) and compared with the isolated atom cross-section (curve A). The increasing shift of the ionization threshold with decreasing  $\lambda_D$  (i.e. with increasing density) clear from the figure 9.

We performed similar calculation for Li-like carbon as well (fig. 10-11). Since there are three bound electrons for these ions, iterative calculations mentioned before was performed for the bound states and the continuum wavefunction was computed with 1-electron removed (by ionization) from the given state 2s or 3s. Comparison



with isolated ion results shows substantial modification of photoionization cross-section at these densities and temperatures and significant shifts of ionization threshold due to effect of the surrounding plasma.

## V. CONCLUSIONS

It is demonstrated that the time-dependent linear response method within the framework of local relativistic density functional theory can provide reliable atomic data for various atoms and ions of experimental interest. This model is particularly useful in those situations where conventional independent particle models fail to provide accurate data. The mechanism of time-dependent polarization of the atom is seen to be important in describing the observed results. As a practical point, the computer code based on the time-dependent model is fast and efficient, capable of generating a large number of data in a short time (for example, cross-sections for 10 photon energies for a medium-Z atom takes about 3 minutes of c.p.u. time on a Cray-XMP computer). The present method is capable of treating large complex atoms with high-Z for which relativistic effects are important. Let us point out that if the applied radiation field strength is very high, so that it is comparable or larger than the atomic field strength, new extensions or developments of the present model is necessary to treat those conditions. Full numerical solution of time-dependent density functional method (beyond the linear response approximation) would be one suitable to use in those cases. Work in this new direction is planned for the future.

With reference to the calculations for the different plasma conditions, let us point out that the Debye-screened form for the long range part of the potential may not be adequate for the high-density plasmas. For more realistic calculation, it is necessary to use fully self-consistent finite temperature density functional method for those plasma conditions. Also, the effect of exchange and correlation for plasma electrons become important at high densities. The present approximate scheme is used at present for computational simplicity. However, the results shown here clearly indicate that with increasing plasma density, the photoionization cross-section and rates of the ions forming the plasma can be substantially modified. Accurate modeling of atomic properties for dense plasmas, therefore, requires that the effect of the surrounding plasma should be properly included in the calculation.

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## Appendix I

The Green's function  $G$  in eq. (11) has 16 components, which are represented in matrix form

$$G(\vec{r}, \vec{r}', E) = \begin{pmatrix} G^{11}(\vec{r}, \vec{r}' | E) & G^{12}(\vec{r}, \vec{r}' | E) \\ G^{21}(\vec{r}, \vec{r}' | E) & G^{22}(\vec{r}, \vec{r}' | E) \end{pmatrix}$$

The angular decomposition of various terms are

$$\begin{aligned} G^{11}(\vec{r}, \vec{r}' | E) &= \sum_{jlm} q_{jlm}(\hat{r}) G_{jl}^{11}(r, r' | E) q_{jlm}^*(\hat{r}') \\ G^{12}(\vec{r}, \vec{r}' | E) &= \sum_{jlm} i^{l-l'} q_{jlm}(\hat{r}) G_{jl}^{12}(r, r', | E) q_{jlm}^*(\hat{r}') \quad (I-2) \\ G^{21}(\vec{r}, \vec{r}' | E) &= \sum_{jlm} i^{l'-l} q_{jl,m}(\hat{r}) G_{jl}^{21}(r, r' | E) q_{jlm}^*(\hat{r}') \\ G^{22}(\vec{r}, \vec{r}' | E) &= \sum_{jlm} q_{jl,m}(\hat{r}) G_{jl}^{22}(r, r' | E) q_{jl,m}^*(\hat{r}') \end{aligned}$$

The radial part  $G^{\alpha\beta}(r, r' | E)$  are solutions of the radial inhomogeneous Dirac equation

$$G_{jl}^{\alpha\beta}(r, r' | E) = \begin{cases} u_{jl}^{\alpha}(r) \bar{u}_{jl}^{\beta}(r') / (rr' W_{jl}) & r < r' \\ u_{jl}^{\alpha}(r) v_{jl}^{\beta}(r') / (rr' W_{jl}) & r > r' \end{cases} \quad (I-3)$$

$W_{jl}$  is the Wronskian

$$W_{jl} = -cS_{jl} [u_{jl}^2(r) \bar{u}_{jl}^1(r) - \bar{u}_{jl}^2(r) u_{jl}^1(r)] = \text{const.}$$

$\bar{u}_{jl}^1(r)$  and  $\bar{u}_{jl}^2(r)$  are major and minor component radial functions that are real and regular at  $r = 0$ .  $\bar{u}_{jl}^1(r)$  and  $\bar{u}_{jl}^2(r)$  major and minor component

radial functions which (for  $E > c^2$ ) are complex and obey outgoing wave boundary conditions at  $r = \infty$ . The phase for  $\bar{u}_{j1}^1$  and  $\bar{u}_{j1}^2$  is chosen so that  $W_{j1}$  is real. When  $E < c^2$ ,  $\bar{u}_{j1}^1(r)$  and  $\bar{u}_{j1}^2(r)$  are real and decay exponentially at large radii.

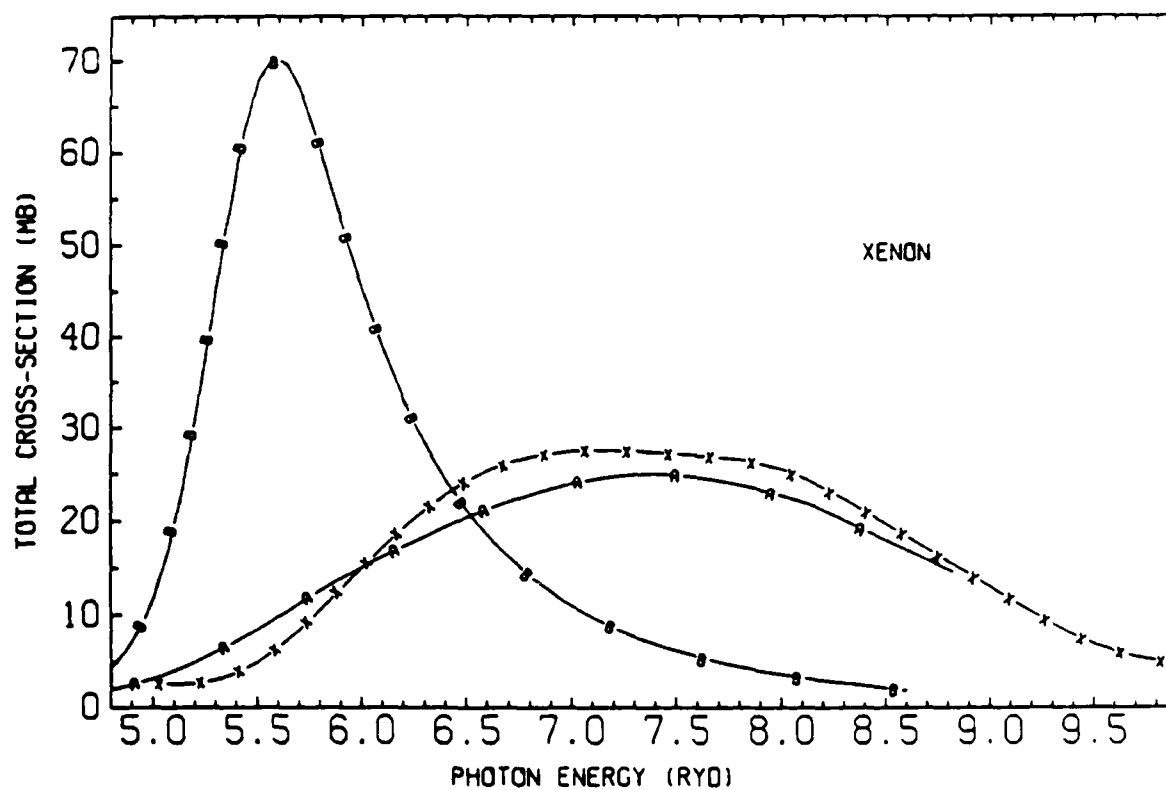
With the above representations, the polarizability  $\chi(r, r'; \omega)$  is given by

$$\begin{aligned} \chi_j(r, r'; \omega) = \sum f_i (2j_2+1) (2l_1+1) (2l_2+1) \times \\ \left[ \begin{pmatrix} l_1 & l_2 & I \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} I & l_1 & l_2 \\ 1/2 & j_2 & j_1 \end{pmatrix} \right]^2 \times \frac{1}{W_{j_2 l_2}(E_i \pm \omega)} \left[ A_i(r) u_{j_2 l_2}^1(r | \epsilon_i \pm \omega) \right. \\ \left. \pm i^{S_1 - S_2} B_i(r) u_{j_2 l_2}^2(r | \epsilon_i \pm \omega) \right] \times \left[ A_i(r') \bar{u}_{j_2 l_2}^1(r' | \epsilon_i \pm \omega) \right. \\ \left. \pm i^{S_2 - S_1} B_i(r') \bar{u}_{j_2 l_2}^2(r' | \epsilon_i \pm \omega) / (rr')^2 \right] \end{aligned} \quad (I-4)$$

when  $r < r'$ ,  $r$  and  $r'$  are interchanged on the right side of eq. (I-4) when  $r > r'$ . The index  $i$  stands for the quantum numbers  $(n, l_1, j_1, S_1)$  of a bound state and  $f_i$  for the occupation factors. The summation is over all indices except  $I$  and over both  $+\omega$  and  $-\omega$ . For the case of  $-\omega$ , the complex conjugates of all outgoing waves in eq. (I-4) are to be used. Angular momentum coupling coefficients are expressed in terms of Wigner  $3j$  and  $6j$  symbols.

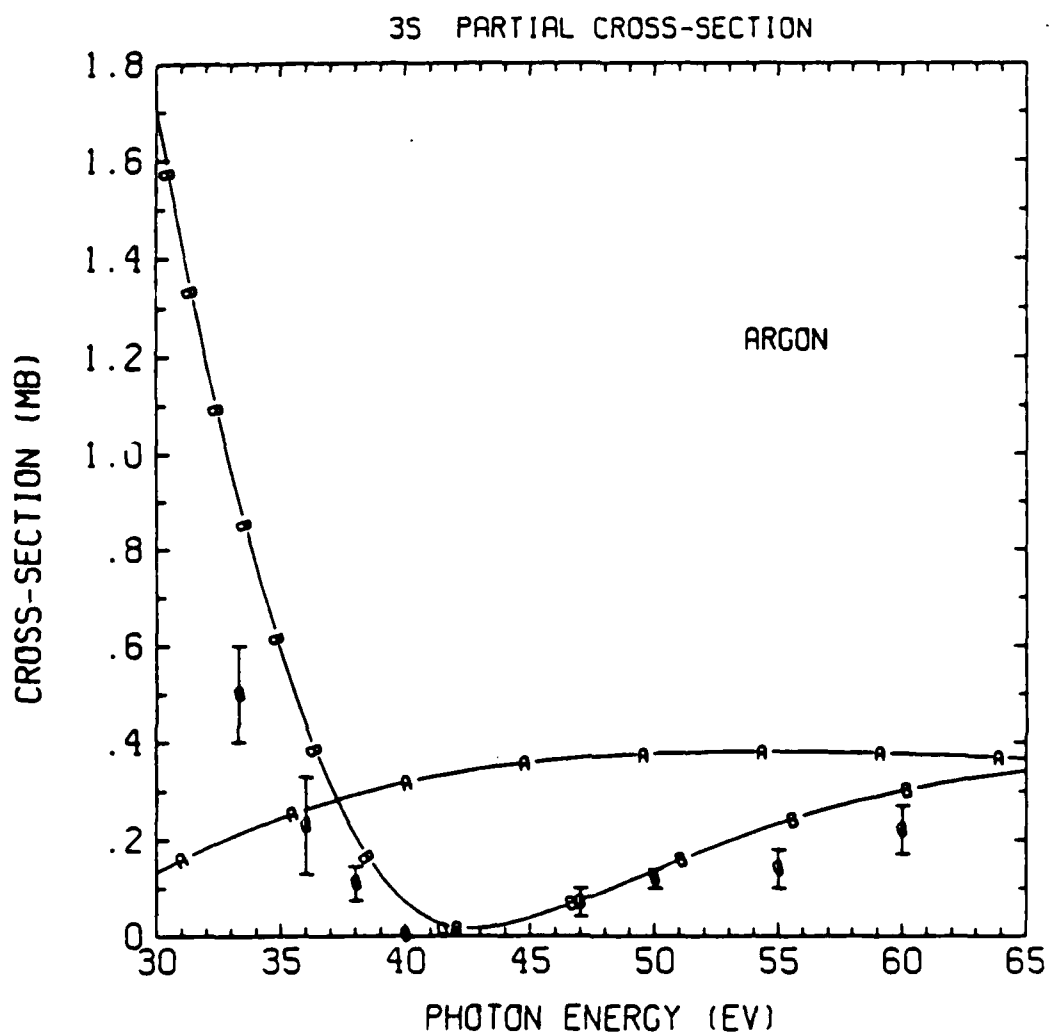
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TOTAL PHOTOIONIZATION CROSS-SECTION OF NEUTRAL XENON NEAR 40 THRESHOLD. CURVE A: TIME DEPENDENT DENSITY FUNCTIONAL CALCULATION. CURVE B: INDEPENDENT PARTICLE MODEL: EXPERIMENTAL DATA FROM R. HANSEL ET. AL., PHYS. REV. 188, 1375 (1969)

Figure 1

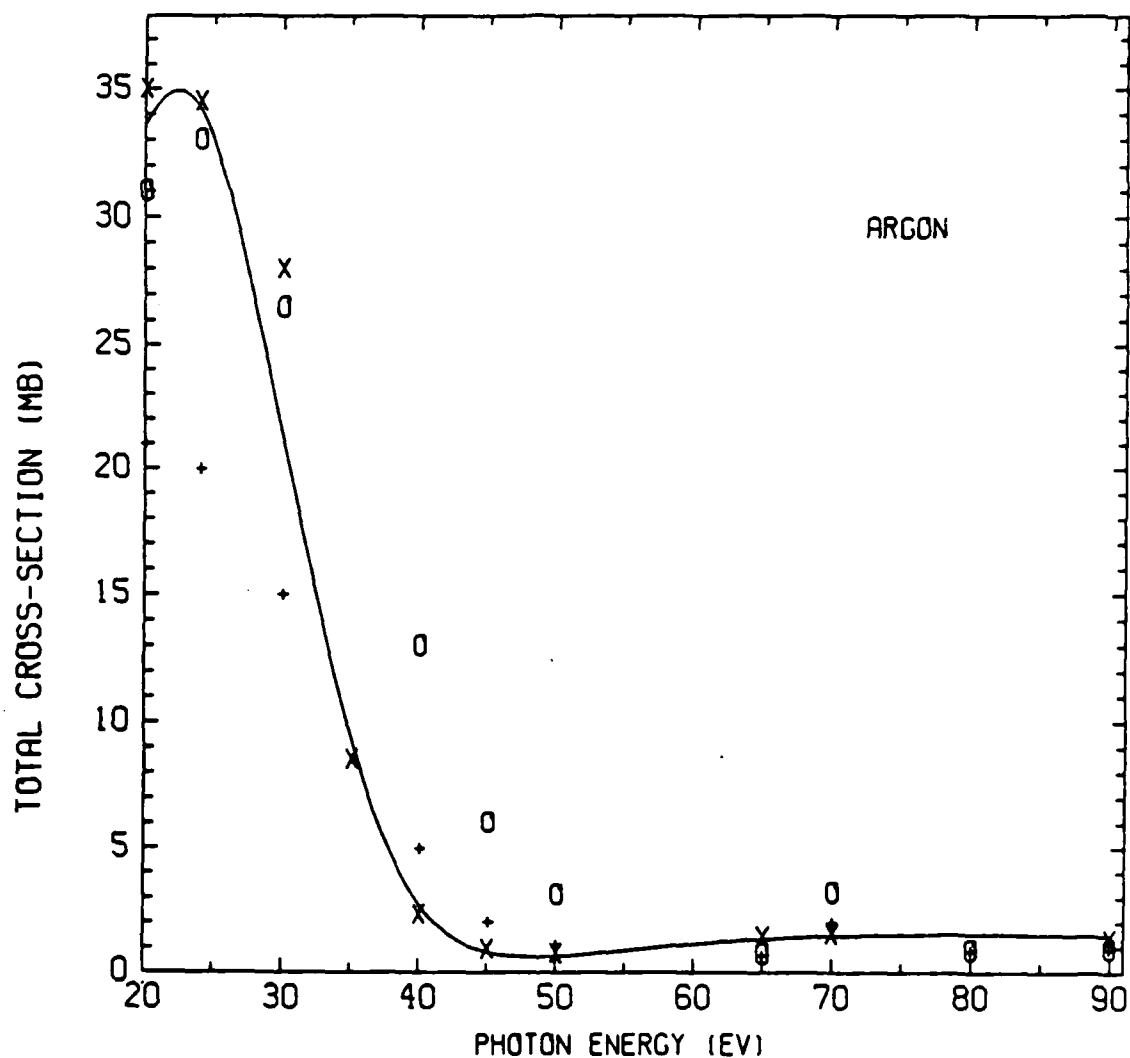


CURVE A: INDEPENDENT PARTICLE MODEL.

CURVE B: TIME-DEPENDENT DENSITY FUNCTIONAL CALCULATION.

DATA FROM K. TAN & C. BRION, J. ELECTRON SPECTROS. 13,  
77(1978).

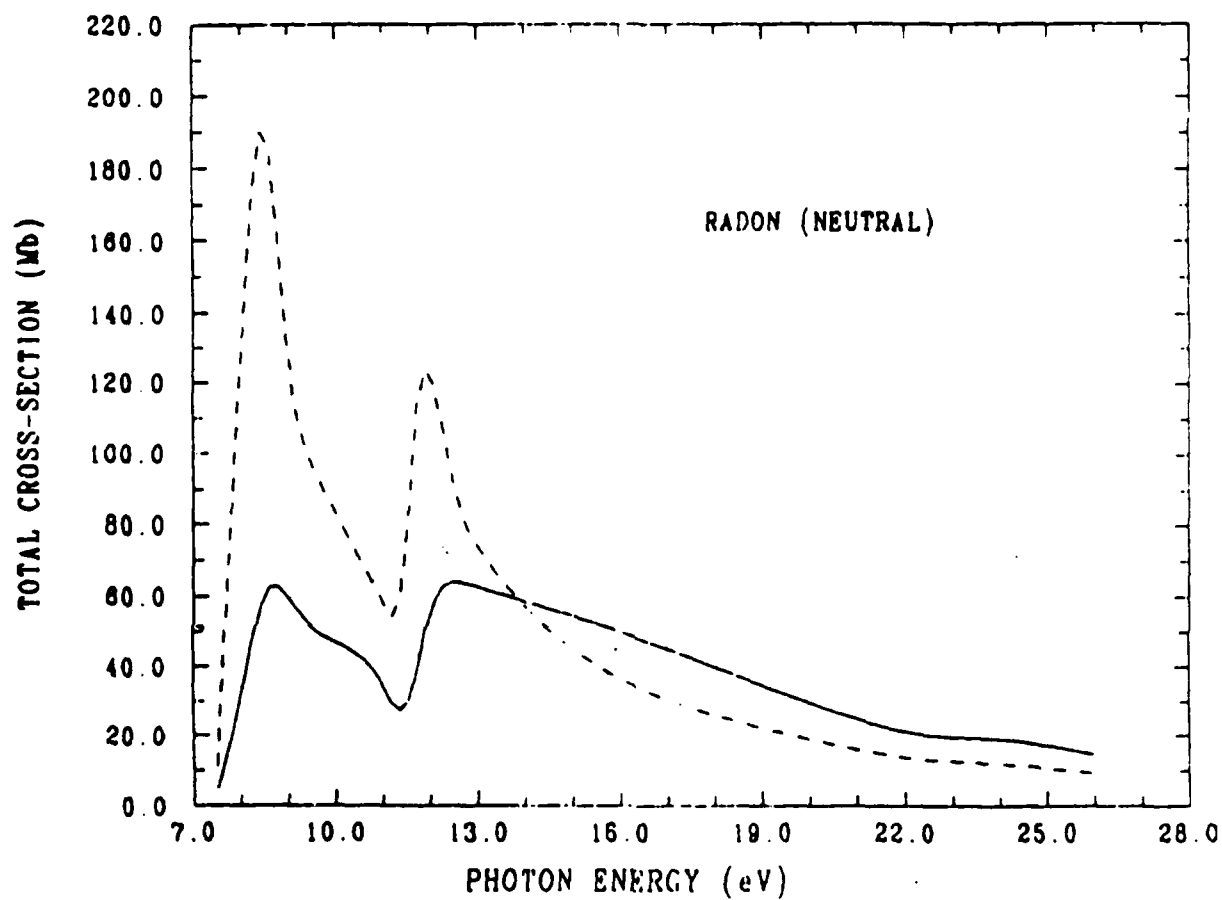
Figure 2



SOLID CURVE: TIME-DEPENDENT DENSITY FUNCTIONAL CALCULATION.  
 X: EXPERIMENTAL DATA FROM J.A.R. SAMSON, ADVAN. ATOM. MOL.  
 PHYS. 2, 178 (1966). +: HARTREE-FOCK (VELOCITY APPROX.) AND  
 O: HARTREE-FOCK (LENGTH APPROX.) BY KENNEDY & MANSON,  
 PHYS. REV. A 5, 227 (1972).

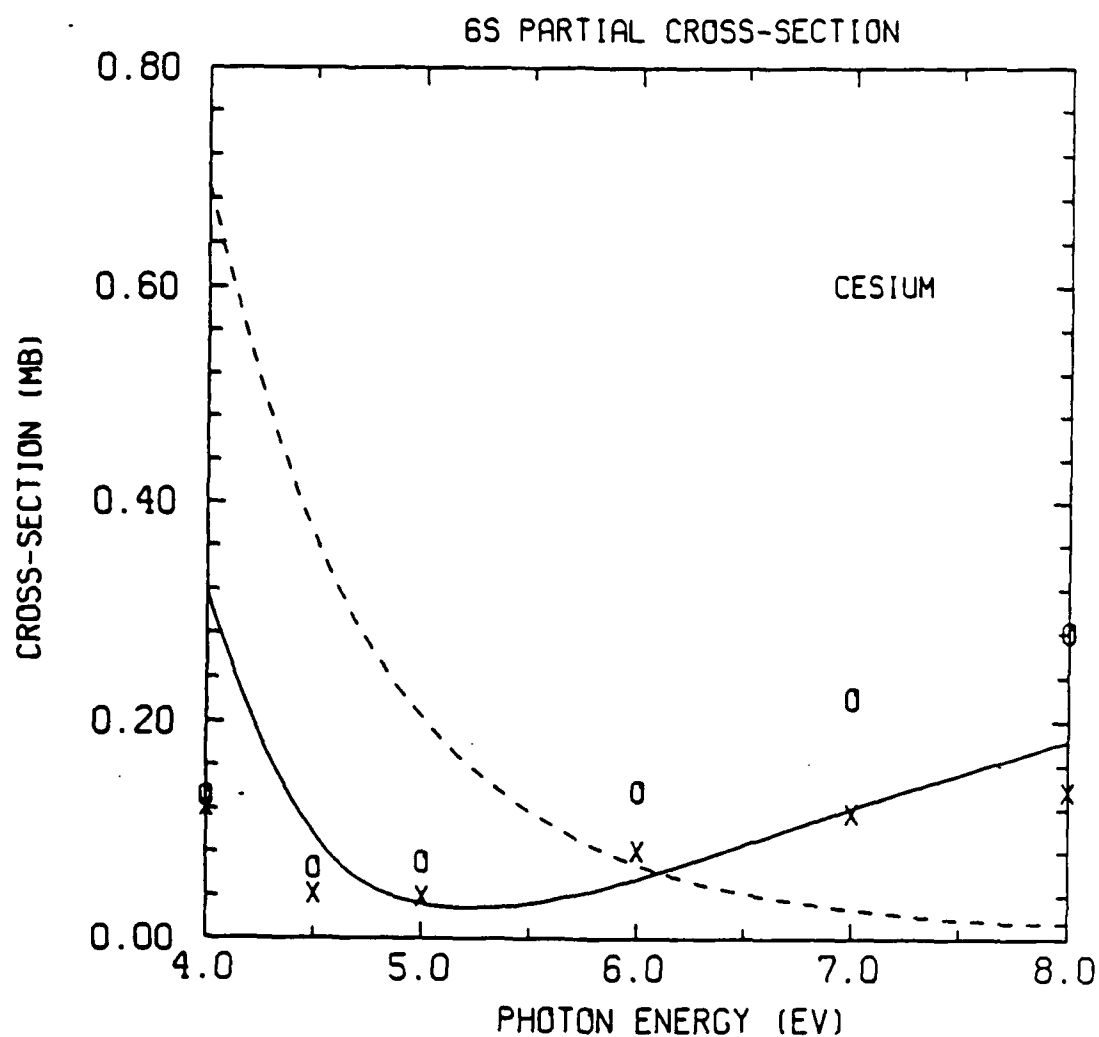
Figure 3





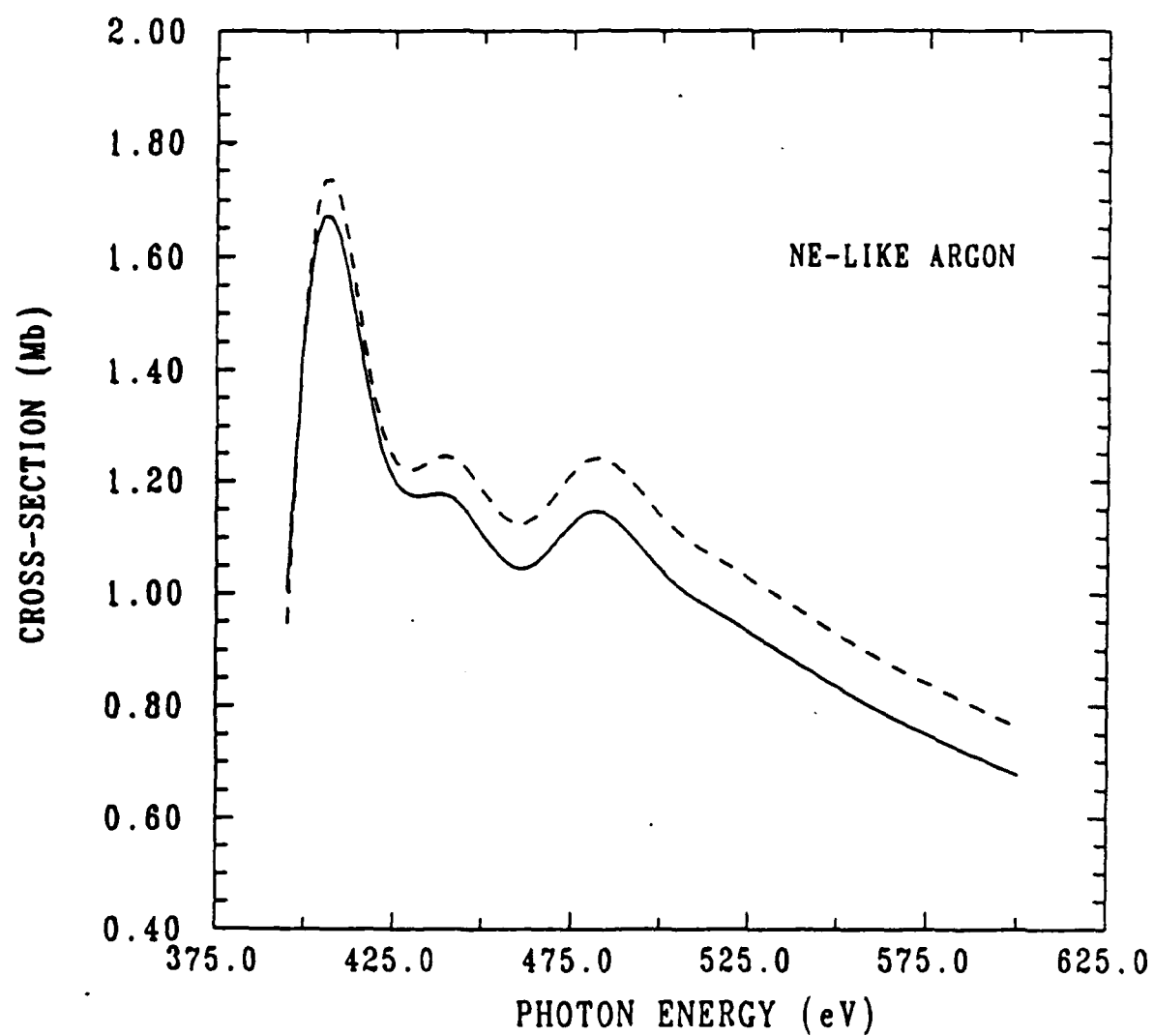
Solid Curve: Time-dependent density functional calculation  
Dashed Curve: Independent particle model

Figure 4



SOLID CURVE: TIME-DEPENDENT DENSITY FUNCTIONAL CALCULATION.  
DASHED CURVE: INDEPENDENT PARTICLE MODEL.  
X: EXPERIMENTAL DATA FROM MOHLER AND BOECKNER, J. RES.  
NBS 3, 303 (1929). O: EXPERIMENTAL DATA FROM MARR AND  
CREEK, PROC. R. SOC. A 304, 233 (1968).

Figure 5



Solid Curve: Independent particle model.

Dashed Curve: Time-dependent density functional calculation.

Figure 6

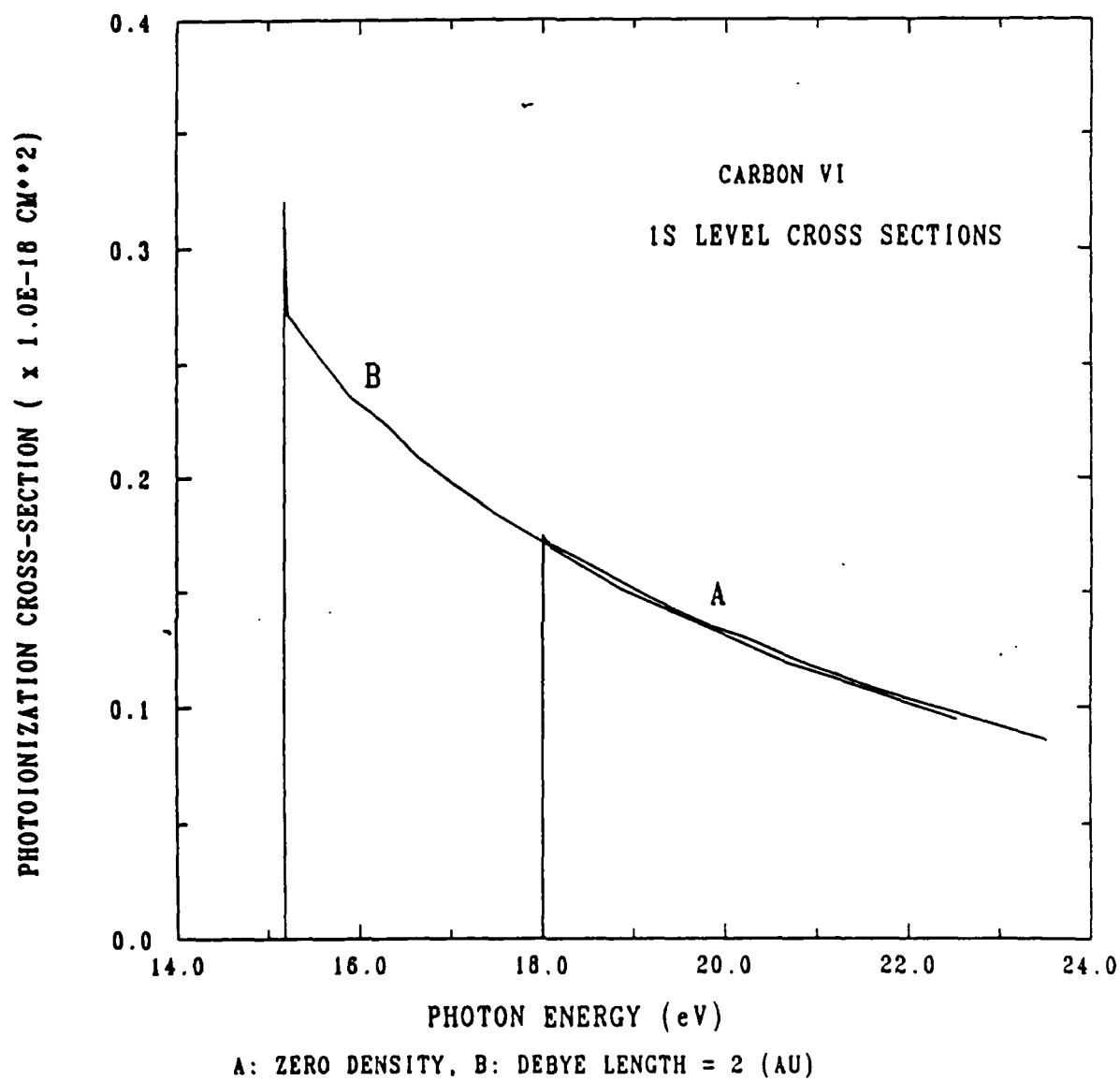
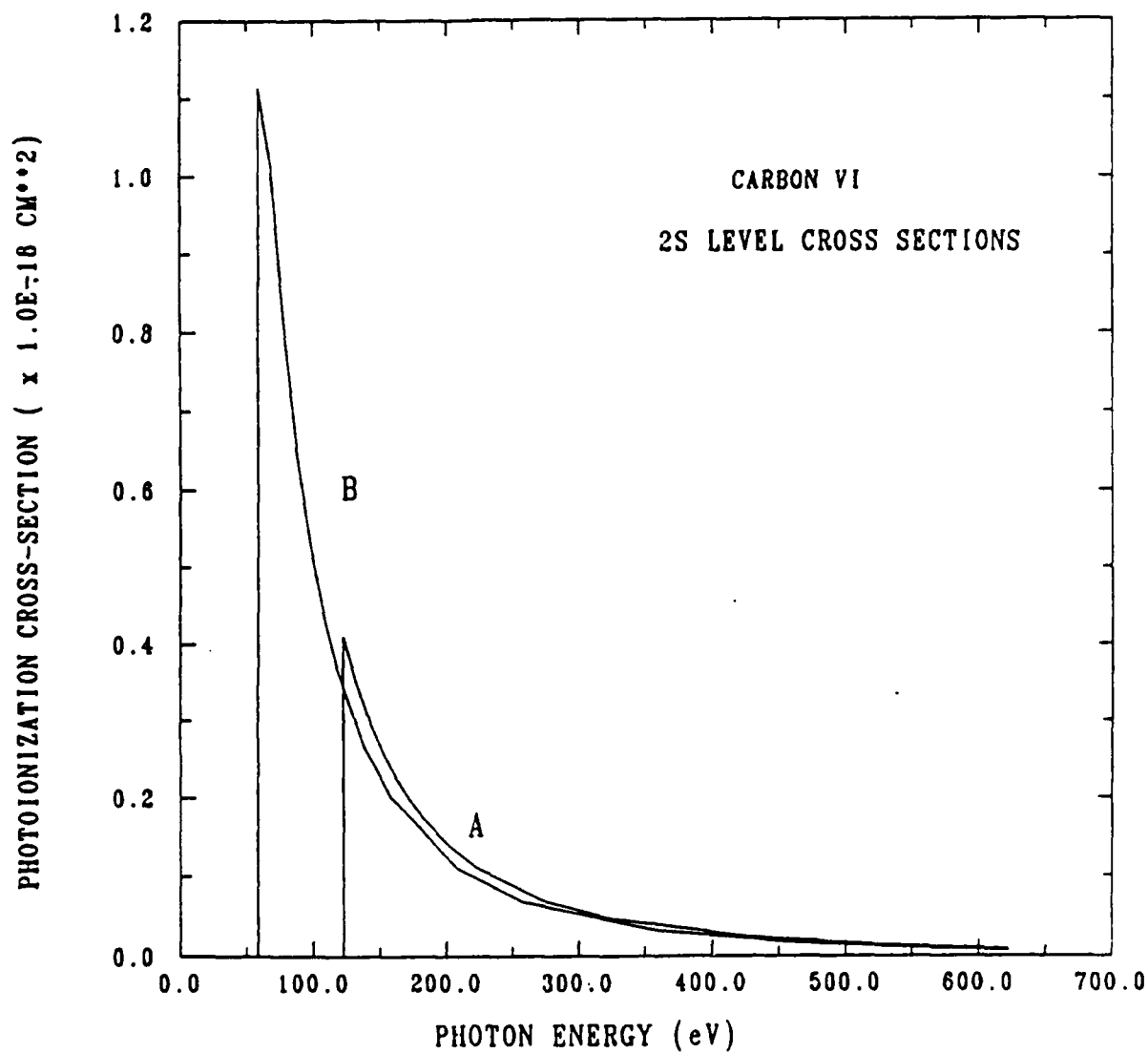


Figure 7



A: ZERO DENSITY, B: DEBYE LENGTH = 2 (AU)

Figure 8

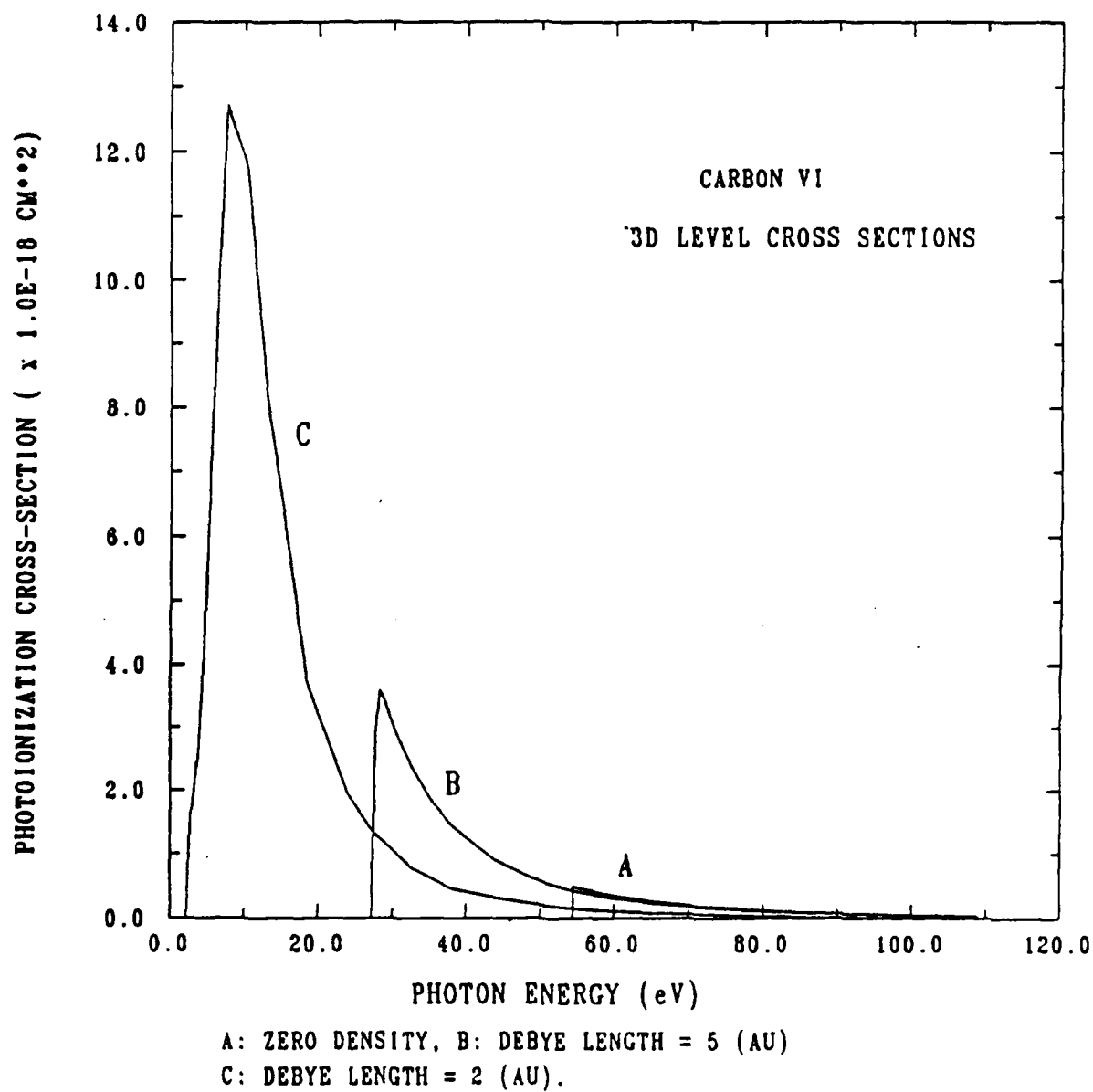


Figure 9

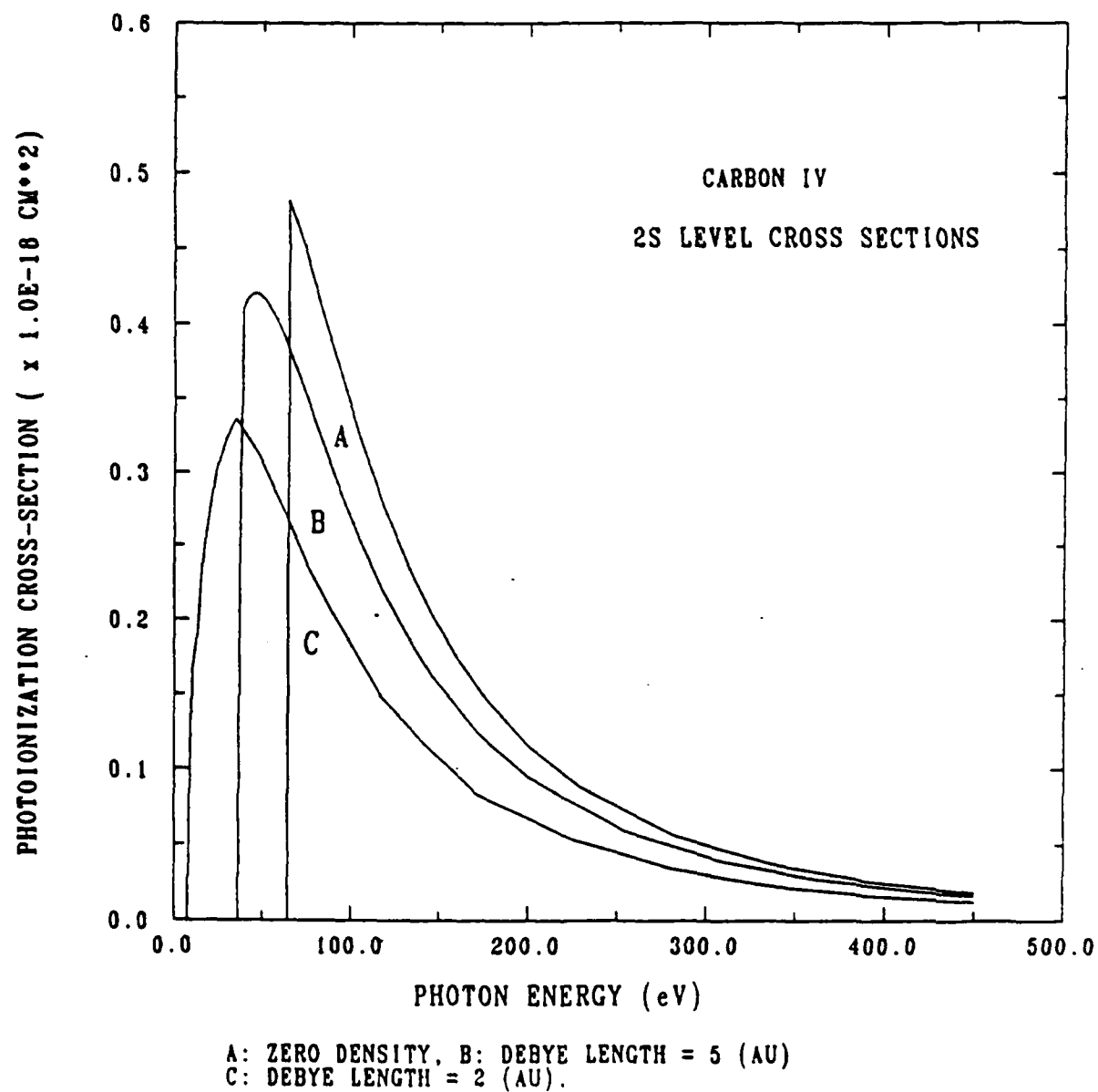


Figure 10

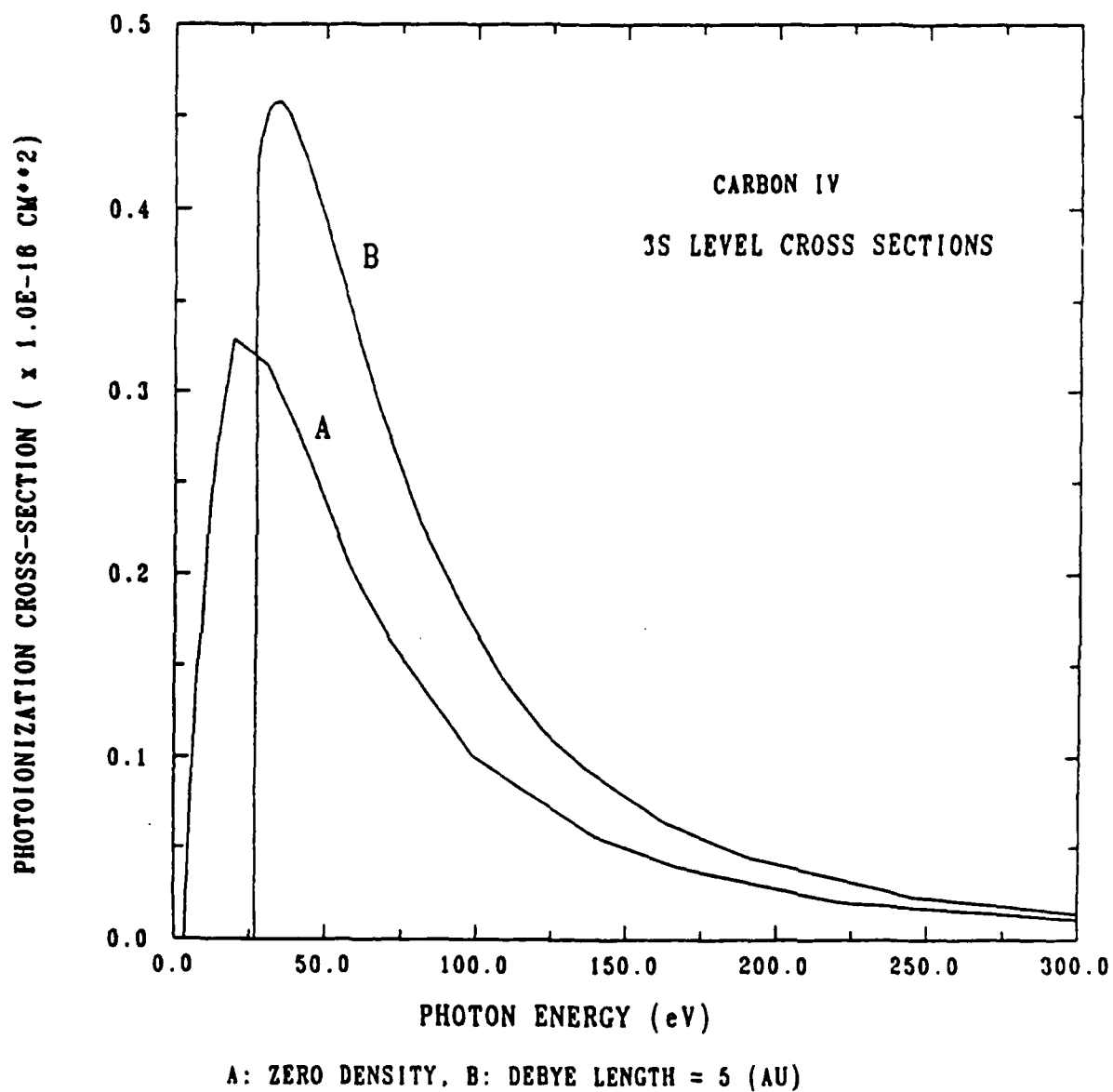


Figure 11



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